

Hierarchy of Spin and Valley Symmetry Breaking in Quantum Hall Single Layer Graphene

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We explore several microscopic mechanisms for breaking the $n = 0$ fourfold Landau level degeneracy in a single-layer graphene. Valley-scattering random potential, Zeeman interaction, and electron-phonon coupling are considered in the presence of SU(4)-symmetric Coulomb exchange interaction. Among all the mechanisms considered, it is the electron-phonon coupling combined with the Zeeman interaction which leads to the full splitting of the $n = 0$ Landau levels. A recent controversy of “valley-first” or “spin-first” breaking of SU(4) symmetry of the $n = 0$ graphene Landau level is examined in light of our results. Existence of midgap states between Landau levels of opposite valley polarity are demonstrated.

PACS numbers: 73.43.Cd, 73.50.-h, 73.61.Wp

Spin and valley degeneracy of a single-layer graphene sheet subject to a perpendicular magnetic field gives rise to a quantized Hall conductance[1, 2] σ_{xy} that changes in multiples of four units of conductance quantum e^2/h : $\sigma_{xy} = 4(e^2/h)(n + 1/2)$, n =integer. The conductance changes from (taking $e^2/h \equiv 1$) -2 to $+2$ as the chemical potential passes through the central, $n = 0$ Landau level (LL) which is fourfold degenerate. When the strength of the magnetic field increases, these fourfold degenerate LL's split in energy into two sublevels[3, 4, 5], and accordingly the Hall conductance steps occur at $-2, 0$, and $+2$. At even higher fields the fourfold degeneracy is broken completely, leading to the sequence $\sigma_{xy} = -2, -1, 0, 1, 2$ [3, 4, 5].

The manner of the breaking of fourfold degeneracy of the central LL has been discussed in a number of papers[6, 7, 8, 9, 10, 11, 12, 13, 14]. The SU(4) symmetry of the pristine $n = 0$ graphene LL is broken down either spontaneously from interaction effects, or due to various weak symmetry-breaking terms such as lattice effects, Zeeman splitting, etc. Since the degeneracy arises from SU(2) symmetry of the electron spin and another SU(2) symmetry of the valley, the main focus of discussion has been whether the spin-symmetry or the valley-symmetry breaking occurs first. Abanin, Levitov, and Lee argued that the spin symmetry breaking should occur first, turning the edge of the Hall sample into conducting channels[7]. An experiment carried out shortly thereafter seems to confirm their picture[4]. On the other hand, subsequent transport experiments[15] which found divergent longitudinal resistance seem to rule out the existence of such gapless edge states, and the issue of “spin-first” or “valley-first” symmetry breaking appears by no means settled.

In this paper, we revisit the “hierarchy problem” of the central LL splitting in a single-layer graphene within the self-consistent Hartree-Fock theory, while considering several SU(4)-symmetry breaking terms explicitly. Following the general approach, we adopt the continuum description of the graphene dynamics using the spinor

$\psi_{\sigma\tau}(r) = \begin{pmatrix} a_{\sigma\tau}(r) \\ b_{\sigma\tau}(r) \end{pmatrix}$. Spin ($\sigma = \uparrow, \downarrow$) and valley index $\tau = \pm$ are introduced to classify the spinors formed from a - and b -sublattice electrons. The Landau level problem with the perpendicular magnetic field can be treated by the Hamiltonian

$$H^K = \hbar\omega_i \sum_{\sigma\tau} \int d^2r \psi_{\sigma\tau}^\dagger(r) \begin{pmatrix} 0 & -a \\ a^+ & 0 \end{pmatrix} \psi_{\sigma\tau}(r). \quad (1)$$

With the non-commuting operators obeying $[p_x, p_y] = i\hbar^2/l_B^2$, $l_B = \sqrt{\hbar/eB}$ being the magnetic length, one can form a set of canonical operators $a = (l_B/\sqrt{2}\hbar)(p_x + ip_y)$, $a^+ = (l_B/\sqrt{2}\hbar)(p_x - ip_y)$, $[a, a^+] = 1$. A cyclotron frequency $\omega = \sqrt{2}v_F/l_B$ (v_F =Fermi velocity) has been introduced above.

In writing down the Hamiltonian in the manifestly SU(4)-symmetric form above, we have implemented the rotation of the $\tau = -$ spinor, $\psi_{\sigma-} \rightarrow \sigma_y \psi_{\sigma-}$. Using the complete set of normalized eigenfunctions given by

$$\chi_{nm} = \frac{1}{\sqrt{2}} \begin{pmatrix} \text{sgn}(n)\phi_{|n|-1,m} \\ i\phi_{|n|m} \end{pmatrix}, \quad \chi_{0m} = \begin{pmatrix} 0 \\ \phi_{0m} \end{pmatrix}, \quad (2)$$

one may expand the field operator as $\psi_{\sigma\tau}(r) = \sum_{n,m} \chi_{nm\tau}(r) \gamma_{nm\sigma\tau}$. Here ϕ_{nm} is the oscillator wave function, m is the guiding center coordinates, and $\chi_{nm\tau}$ equals χ_{nm} defined in Eq. (2) if $\tau = +$, but equals $\sigma_y \chi_{nm}$ when $\tau = -$.

As the primary interest of this paper is in understanding the mechanism of level splitting within the central LL, we carry out the projection to $n = 0$ LL states. The kinetic energy gets completely quenched, whereas Coulomb interaction within this LL reads

$$H^C = \frac{1}{2} \int_{rr'} V(r-r') \phi_{m_4}^*(r) \phi_{m_1}(r) \phi_{m_3}^*(r') \phi_{m_2}(r') \\ \times \sum_{\sigma\sigma'\tau\tau'} \gamma_{m_4\sigma\tau}^+ \gamma_{m_3\sigma'\tau'}^+ \gamma_{m_2\sigma'\tau'} \gamma_{m_1\sigma\tau}. \quad (3)$$

The reference to the LL index $n = 0$ has been dropped. The summation over the repeated guiding center coordinates is implicit. For numerical purpose, we work with a torus geometry of dimension $L_x \times L_y$ and use the Landau gauge for which the wave functions are

$$\phi_m(r) = \frac{1}{\pi^{1/4} L_x^{1/2}} e^{iy_m x} e^{-\frac{1}{2}(y-y_m)^2}, y_m = \frac{2\pi}{L_x} m. \quad (4)$$

The Coulomb Hamiltonian in this basis reads

$$H^C = \frac{1}{2} \frac{1}{L_x L_y} \sum_{k_x, k_y} V(k_x, k_y) e^{-\frac{1}{2}k_x^2 - \frac{1}{2}k_y^2 + ik_y(y_{m_1} - y_{m_2} + k_x)} \times \sum_{\sigma\sigma'\tau\tau'} \gamma_{m_1+m_x\sigma\tau}^+ \gamma_{m_2-m_x\sigma'\tau'}^+ \gamma_{m_2\sigma'\tau'} \gamma_{m_1\sigma\tau}, \quad (5)$$

where the Fourier-transformed Coulomb potential $V(k) = \int d^2r V(r) e^{ik \cdot r}$ is shown. Whereas k_x, k_y run over all integer multiples of $2\pi/L_x$ and $2\pi/L_y$, the guiding center coordinates m_1 and m_2 span 1 through N_ϕ , the number of flux through the lattice N_ϕ given by $2\pi N_\phi = L_x L_y$.

Having established a discretized Hamiltonian, we solve it within the Hartree-Fock theory using the self-consistent parameter

$$\Delta_{\sigma_1\tau_1, \sigma_2\tau_2}(m_1, m_2) = \langle \gamma_{m_1\sigma_1\tau_1}^+ \gamma_{m_2\sigma_2\tau_2} \rangle \quad (6)$$

with an arbitrary pair of guiding center indices m_1, m_2 and the spin-valley indices. For the reason that Hartree term offers only a chemical potential shift for the uniform solutions we find, and that Hartree interaction does not break the SU(4) symmetry, we will be exclusively concerned with the exchange Hamiltonian, H^{EX} .

Among the possible SU(4) symmetry-breaking terms we consider the following three: (i) Zeeman field: $H^B = B_\sigma \sum_{m\sigma\tau} \sigma \gamma_{m\sigma\tau}^+ \gamma_{m\sigma\tau}$, (ii) Valley-scattering impurity: $H^{\text{imp}} = \sum_{m\sigma\tau} V_m \tau \gamma_{m\sigma\tau}^+ \gamma_{m\sigma\tau}$. We take V_m as a random number of width W : $V_m \in [-W/2, W/2]$, and (iii) Valley-scattering electron-phonon coupling[16]: $H^{\text{el-ph}} = -U \int_r \sum_{\sigma\sigma'\tau} (\psi_{\sigma\tau}^\dagger \sigma_x \psi_{\sigma\bar{\tau}}) (\psi_{\sigma'\bar{\tau}}^\dagger \sigma_x \psi_{\sigma'\tau})$ ($\bar{\tau} = -\tau$). Projected onto the central LL and treated in the mean-field manner, this last Hamiltonian becomes

$$H_{\text{MF}}^{\text{el-ph}} = -U' \sum_{m\sigma\tau} \left(\sum_{\sigma'} \Delta_{\sigma'\tau, \sigma'\bar{\tau}}(m, m) \right) \gamma_{m\sigma\tau}^+ \gamma_{m\sigma\tau}, \quad (7)$$

where $U' = U/\sqrt{2\pi}$ [17]. For convenience, we use U instead of U' from now.

The total Hamiltonian we will consider is $H = H^{\text{EX}} + H^B + H^{\text{imp}} + H_{\text{MF}}^{\text{el-ph}}$. Although all these terms individually may have been analyzed in various ways in the past, it is our belief that their combined effects and possible competition among different symmetry-breaking tendencies have never been studied in the presence of the

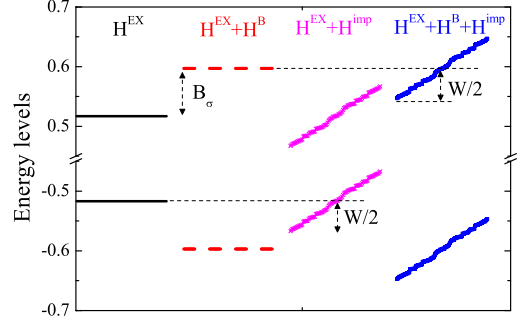


FIG. 1: (color online) Plot of energy levels at half-filling obtained from self-consistent solutions of H^{EX} (black solid lines), $H^{\text{EX}} + H^B$ (red dash lines), $H^{\text{EX}} + H^{\text{imp}}$ (magenta crosses), and $H^{\text{EX}} + H^B + H^{\text{imp}}$ (blue filled squares). The impurity broadening is $W = 0.1$ and the Zeeman field is $B_\sigma = 0.08$. The system size used is $N_\phi = 50$.

Coulomb exchange interaction in a self-consistent manner. We made extensive numerical simulation at zero temperature to identify which of the combinations of the Zeeman, impurity, and electron-phonon coupling-induced interactions would lead to the full splitting of the four-fold degeneracy. Both quarter-filled and half-filled cases were examined. The 3/4-filled case can be deduced by symmetry from the results of 1/4-filled case.

With H^{EX} alone and at half-filling, the initial four-fold degeneracy of the LL is split into two sublevels with energies at $\pm E^{\text{EX}}$, where the scale E^{EX} is set by the exchange energy interaction. In our convention, $e^2/\kappa l$ (κ =dielectric constant) is taken to unity, and in such a unit we obtain $E^{\text{EX}} \approx 0.5$. For the quarter-filled case, a similar situation arises with one LL at an energy below the chemical potential and three degenerate LL's whose energy lies above it. From these exercises we learn that the full energy splitting of the central LL requires more than the Coulomb exchange effect alone. Which of the spin and valley symmetry remains intact is completely arbitrary at this point.

Still at half-filling, inclusion of the Zeeman field to the Coulomb exchange now ensures that the symmetry breaking occurs along the spin direction, with the LL energies at $\pm(E^{\text{EX}} + B_\sigma)$. The valley-SU(2) symmetry is preserved under the addition of H^B . It thus appears that more than one SU(4) symmetry breaking mechanism need to be present to fully split the degeneracy. We find that further inclusion of the valley-scattering impurity, $H^{\text{EX}} + H^B + H^{\text{imp}}$, does not result in additional splitting of the levels. The previously twofold degenerate states for each guiding center m undergoes splitting by $\pm V_m$, and give rise to broadened energy levels of width W . The numerically obtained energy levels for several combinations of terms at half-filling can be found in Fig. 1.

Actually, the Coulomb exchange Hamiltonian per-

turbed by two kinds of Zeeman fields separately acting on the spin and the valley spaces, as in $H^{\text{EX}} + B_\sigma \sum_{m\sigma\tau} \sigma \gamma_{m\sigma\tau}^+ \gamma_{m\sigma\tau} + B_\tau \sum_{m\sigma\tau} \tau \gamma_{m\sigma\tau}^+ \gamma_{m\sigma\tau}$, does exhibit a full lifting of the fourfold degeneracy with the energies given at $(E^{\text{EX}} + B_M) \pm B_m$ and at $-(E^{\text{EX}} + B_M) \pm B_m$. Here B_M and B_m refer to the larger and the smaller of the two Zeeman fields, respectively. One can also see that the electron-phonon coupling $H_{\text{MF}}^{\text{el-ph}}$ provides the required valley Zeeman field, acting along the x -axis of the valley spin.

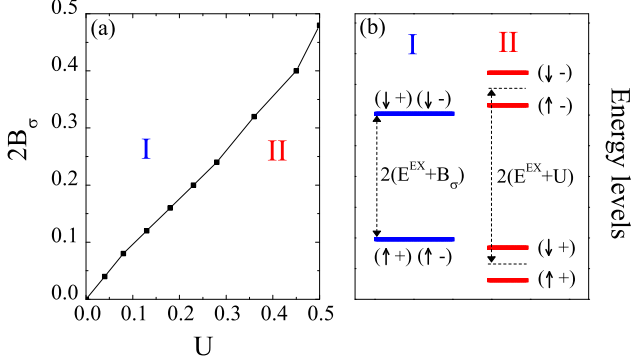


FIG. 2: (color online) (a) Phase diagram of the central LL at half-filling with varying Zeeman field ($2B_\sigma$) and electron-phonon coupling strength (U). In region I, only the spin degeneracy is broken. In region II, both spin and valley symmetries are lost, but the main level splitting takes place in the valley direction. A first-order phase boundary separates the two regions. (b) Schematic energy levels in each region. The energy level separations and spin-valley quantum numbers for each LL are specified.

Aided by these ideas, we next consider $H^{\text{EX}} + H^{\text{B}} + H_{\text{MF}}^{\text{el-ph}}$. Figure 2 shows the phase diagram for such a model, at half-filling, spanned by two interaction parameters ($U, 2B_\sigma$). There are two phases found here, called I and II, distinguished by the number of levels split. In region I, where the Zeeman effect dominates, only one, spin-polarized level splitting is observed. The valley-splitting order parameter $\Delta_{\sigma-, \sigma+}(m, m)$ becomes zero in this region, still preserving the valley symmetry. In the U -dominated region II, the main polarization direction is along the valley axis, and the Zeeman field contributes to the sublevel splitting equal to $2B_\sigma$. Here indeed, the full breaking of the fourfold degeneracy is obtained. The phase boundary taking place along $2B_\sigma \approx U$ in the phase diagram is first-order.

The phase diagram for quarter-filling is similar, as shown in Fig. 3. The phase boundary now taking place exactly at $2B_\sigma = U$ separates the “spin-first”-split region I from the “valley-first”-split region II. The two centrally located LL’s cross in energy at the phase boundary. For instance, $E(\uparrow, -) < E(\downarrow, +)$ energy hierarchy in region I crosses over to $E(\uparrow, -) > E(\downarrow, +)$ in region II. We have checked that the inclusion of the impurity does not alter

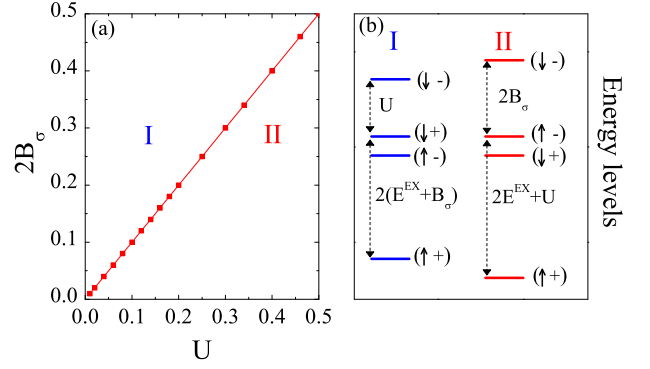


FIG. 3: (color online) Phase diagram of the central LL at quarter-filling. Meaning of the symbols are the same as in Fig. 2. Only one LL lies below the Fermi level here.

the basic features of the phase diagram shown in Figs. 2 and 3 as long as W remains small compared to both U and $2B_\sigma$.

The relevant energy scales $2B_\sigma$ and U in a graphene layer are comparable, as recently discussed in Ref. [16]. Both energy scales are of order B_σ in units of [Kelvin/Tesla], and therefore it should be quite possible that graphene samples with either $2B_\sigma > U$ or $2B_\sigma < U$ exist. Then according to Ref. [7], the edge of the half-filled graphene quantum Hall system can be either conducting ($U < 2B_\sigma$) or insulating ($U > 2B_\sigma$). Another interesting possibility suggested by our search is the transition between the two LL splitting scenarios driven by the relative strengths of electron-phonon coupling and Zeeman energies. We speculate that applying a mechanical pressure, such as stretching, to the graphene will influence U without changing the Zeeman energy, and might allow one to probe the phase transition between regions I and II. The bond-CDW order associated with region II at half-filling and regions I and II for quarter-filling should leave a mark in the electronic spectrum, which can be probed by STM.

A Landau level with a quantum number (σ, τ) occurs at the same energy as another state with $(\sigma, \bar{\tau})$, whereas the same is not true with $(\bar{\sigma}, \tau)$ due to the Zeeman splitting. One can then imagine domain walls separating the two LL states with opposite valley polarities in a macroscopic sample. Assuming the spinless case for simplicity, the physics of such a domain wall can be captured in a set of differential equations

$$\begin{aligned} i(\partial_y + y_k)[u_- + v_+] + m_v(y)[u_+ - v_-] &= -\varepsilon_k[u_+ - v_-] \\ i(\partial_y - y_k)[u_+ - v_-] - m_v(y)[u_- + v_+] &= -\varepsilon_k[u_- + v_+] \\ i(\partial_y + y_k)[u_- - v_+] + m_v(y)[u_+ + v_-] &= \varepsilon_k[u_+ + v_-] \\ i(\partial_y - y_k)[u_+ + v_-] - m_v(y)[u_- - v_+] &= \varepsilon_k[u_- - v_+]. \end{aligned} \quad (8)$$

We have written the eigenfunction associated with the a - and b -sublattice as (u_τ, v_τ) , also distinguished by their

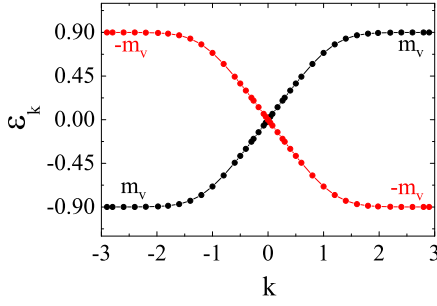


FIG. 4: (color online) The energy ε_k obtained from Eq. (9) with $m_v = 0.9$.

valley index τ , used the linear gauge ($A_x = -By, A_y = 0$), and taken out the x -dependence of the wave function as $(u_\tau, v_\tau) \rightarrow e^{ikx}(u_\tau(y), v_\tau(y))$. The y -dependent mass gap due to the inter-valley scattering is written $m_v(y)$, and y_k abbreviates $y - k$.

As an example of the influence of the sign change of the mass gap on the energy spectra, consider the case with an abrupt sign change as in $m_v(y) = m_v \text{sgn}(y)$. Away from $y = 0$ the mass gap is uniform, and a pair of solutions with $\varepsilon_k = \pm m_v$ is found for $u_+ = v_- = 0$, and $u_- = \pm v_+ = \phi(y - k)$ respectively, where $\phi(y - k)$ is the Gaussian function peaked at $y = k$. Since k is still a good quantum number, the eigen energies ε_k can be solved for each k separately. By matching the wave functions at $y = 0$ we derive the following equation determining the energies,

$$\frac{m_v - \varepsilon_k}{m_v + \varepsilon_k} = \frac{H(p_k, k)H'(p_k, -k)}{H(p_k, -k)H'(p_k, k)}, \quad (9)$$

where $p_k = (\varepsilon_k^2 - m_v^2)/2 < 0$, and $H(p_k, k)$ is Hermite polynomial of negative order p_k . Self-consistently solving the equation for each k gives rise to the energy band shown in Fig. 4.

The level crossing predicted here will be of particular relevance if the chemical potential should lie between the two valley-split LL's. In such a case, a pair of gapless one-dimensional channels will cross the Fermi level, similar to the edge channel in the spin-split case first discussed in Ref. [7]. Unlike the edge channels, the metallic channel predicted here can be formed at the bulk whenever a domain boundary separates the opposite valley states. Referring to our phase diagram in Fig. 2, the two LL's lying closest to the Fermi level always carry opposite spins, therefore a domain wall state connecting the occupied and the unoccupied LL's will have to involve twist in both spin and valley. On the other hand, the quarter-filled case (region I) offer a better chance for observing the domain wall between two spin-polarized LL's which differ only in their valley polarities. We therefore suggest that the "spin-first" split LL with $\sigma_{xy} = -1$ is the most likely platform to observe the metallic domain

walls.

In summary, we explored the hierarchy issue of the central LL symmetry breaking of a graphene layer. Self-consistent Hartree-Fock theory was employed, taking into consideration several kinds of SU(4) symmetry breaking terms. The competitive nature of the valley-splitting (due to electron-phonon interaction) and spin-splitting (due to Zeeman interaction) leads to a phase diagram with either "spin-first" or "valley-first" level splitting. Existence of a new kind of gapless state when LLs with opposite valley polarities form a domain wall is demonstrated.

H. J. H. is supported by the Korea Science and Engineering Foundation (KOSEF) grant funded by the Korea government (MEST) (No. R01-2008-000-20586-0), and in part by the Asia Pacific Center for Theoretical Physics. One of us (H. J. H.) wishes to thank P. Kim for hospitality during the completion of this work and for discussion.

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